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Short communication

Ultra large-scale simulation of polymer electrolyte fuel cells

Yun Wang, Chao-Yang Wang *

Electrochemical Engine Center (ECEC), and Department of Mechanical and Nuclear Engineering, The Pennsylvania State University, University Park, PA 16802, USA

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Abstract

This paper reports on the computational performance and detailed results of ultra large-scale simulations of a 200 cm^2 polymer electrolyte fuel cell (PEFC) using a 23.5 million gridpoint mesh. The computer code is based on a comprehensive single-phase PEFC model that features a detailed membrane-electrode assembly (MEA) model, electron transport, thermal and species transport, coolant heat transfer, in addition to other standard functionalities. Two cases under dry operation are simulated and compared. One case concerns an infinitely large coolant flowrate and consequently a constant temperature of bipolar plates. The other case involves a finite flowrate and a lower inlet coolant temperature designed to avoid membrane dryout in the inlet region while alleviating electrode flooding in the outlet region.
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Keywords: Computational fuel cell dynamics; Polymer electrolyte fuel cells; Large-scale simulation; Cooling

1. Introduction

Computer simulation of PEFCs has been an active research area: see the most recent comprehensive review of Wang [1]. Significant capabilities exist using the single-phase modeling approach. Notable examples include a detailed model of membrane-electrode assembly (MEA) [2–4], electron transport and direct prescription of constant current boundary condition [5,6], non-isothermal modeling and hence coupled consideration of water and thermal management [7], variable gas flow [8,9], transient analysis [10], and experimental validation against detailed current distribution data [11,12].

For single-phase calculations, Meng and Wang [13] first proposed a parallel computing methodology to handle large-scale simulations involving millions of gridpoints. They simulated a variety of wet-to-dry operating conditions with a five-channel serpentine flow-field and benchmarked the parallel computing performance to be greater than 7 × speed-up with 10 processors. The largest calculations reported so far were by Wang [1] (2.7 million cells); Shimpalee et al. [14] (5 million cells), and Wang and Wang [15] (2.7 million cells). However, the industry has a need for simulations using an order-of-magnitude larger mesh with reasonable computing time. This paper presents 23.5 million gridpoint calculations for the first time, herein termed ultra large-scale simulation to distinguish from prior studies of large-scale simulations. In addition, we will show a capability to perform co-simulation of electrochemical/transport phenomena in a PEFC and heat transfer in coolant channels. Such an integrated heat and water management tool is highly desirable in design and engineering of commercial-size PEFCs.

2. Numerical model

Fig. 1 shows the computational domain of the 200 cm^2 PEFC featuring a 24-channel, 3-pass serpentine flowfield, which includes the flow plates, gas and coolant channels, gas diffusion layers (GDLs), and catalyst layers on both the anode and cathode, as well as the membrane. The geometrical dimensions of various components in the cell are listed in Table 1.

* Corresponding author. Tel.: +1 814 863 4762; fax: +1 814 863 4848.
E-mail address: cxw31@psu.edu (C.-Y. Wang).

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Nomenclature

c_p	specific heat ($J\,kg^{-1}\,K^{-1}$)
C_k	molar concentration of species k ($mol\,m^{-3}$)
D	mass diffusivity of species ($m^2\,s^{-1}$)
F	Faraday's constant (96,487 $C\,eq.^{-1}$)
I	current density ($A\,cm^{-2}$)
K	permeability (m^2)
P	pressure (Pa)
R	gas constant ($8.134\,J\,mol^{-1}\,K^{-1}$)
S	source term in transport equations
T	temperature (K)
$\vec{u}$	velocity vector ($m\,s^{-1}$)

Greek letters

α	net water transport coefficient per proton
ε	porosity
ϕ	phase potential (V)
κ	ionic conductivity ($S\,m^{-1}$)
λ	membrane water content, $\#H_2O/\#SO_3^-$
ρ	density ($kg\,m^{-3}$)
σ	electronic conductivity ($S\,cm^{-1}$)
τ	shear stress ($N\,m^{-2}$)
ξ	stoichiometric flow ratio

Superscripts and subscripts

a	anode
avg	average
c	cathode
e	electrolyte
eff	effective value
g	gas phase
k	species
m	membrane
s	electronic phase
sat	saturate value
w	water

2.1. Governing equations

The single-phase PEFC model employed in this work consists of nonlinear, coupled partial differential equations governing the conservation of mass, momentum, species, energy, and charge with electrochemical reactions. The equations can be written in the vector form, as [3–7]:

$$\text{Continuity equation}: \quad \nabla\cdot(\rho\vec{u}) = 0 \tag{1}$$

Momentum conservation :

$$\frac{1}{\varepsilon^2}\nabla\cdot(\rho\vec{u}\vec{u}) = -\nabla p + \nabla\cdot\tau + S_{\mathrm{u}} \tag{2}$$

$$\text{Species conservation}: \quad \nabla\cdot(\vec{u}C_k) = \nabla\cdot(D_k^{\mathrm{eff}}\nabla C_k) + S_k \tag{3}$$

$$\text{Energy conservation}: \quad \nabla\cdot(\rho c_p\vec{u}T) = \nabla\cdot(k^{\mathrm{eff}}\nabla T) + S_{\mathrm{T}} \tag{4}$$

$$\text{Proton transport equation}: \quad \nabla\cdot(\kappa^{\mathrm{eff}}\nabla\phi_{\mathrm{e}}) + S_{\phi_{\mathrm{e}}} = 0 \tag{5}$$

$$\text{Electron transport equation}: \quad \nabla\cdot(\sigma^{\mathrm{eff}}\nabla\phi_{\mathrm{s}}) + S_{\phi_{\mathrm{s}}} = 0 \tag{6}$$

where ρ, $\vec{u}$, p, C_k, T, ϕ_{e}, and ϕ_{s} denote the gas density, superficial fluid velocity vector, pressure, molar concentration of species k, temperature, electrolyte and electronic phase potentials, respectively. The species considered here are hydrogen, oxygen, and water. The various source terms, electrochemical properties, and thermophysical properties identified for various regions of a PEFC, as well as necessary boundary conditions, have been detailed in [3–7] and thus are not repeated here. Select physical properties most relevant to the present simulation results are listed in Table 1.

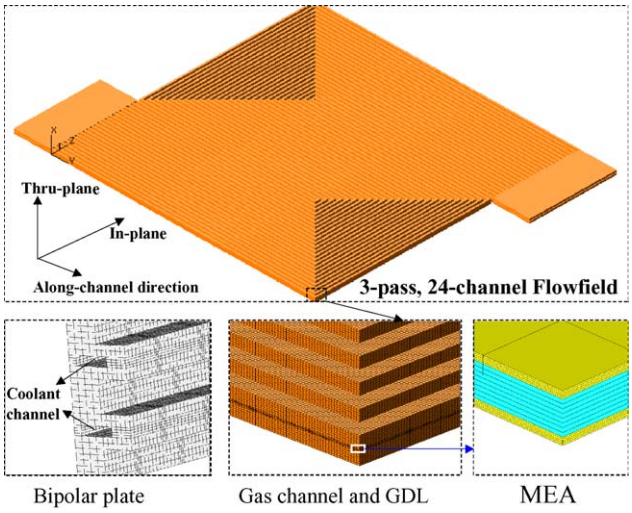

Fig. 1. Computational domain and mesh of a 200 cm^2 PEFC.

2.2. Numerical procedure

The conservation equations, Eqs. (1)–(6), are solved by the commercial package, Fluent®, with the SIMPLEC algorithm [16], using a parallel computational methodology for a Linux PC cluster. The SIMPLEC algorithm is to update the pressure and velocity fields from the solution of the pressure corrections equation, solved by algebraic multigrid (AMG) method [17]. Following the solution of the flow field, the energy, species, proton, and electron equations are solved. Approximately 23.5 million computational elements ($46\times900\times600$) are employed to capture details of flow, thermal, electrochemical and mass transport phenomena in the PEFC. The MEA, where the important electrochemical

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